



FIVE DAY INTERNATIONAL WORKSHOP-CUM-SEMINAR

on

ARTIFICIAL INTELLIGENCE IN CHEMISTRY & RECENT TRENDS IN CHEMISTRY RESEARCH

organized by

DEPARTMENT OF CHEMISTRY, NSCBM GOVERNMENT COLLEGE HAMIRPUR

in collaboration with

E-Cell Make Intern, IIT Hyderabad
(10th November to 14th November 2025)





PROGRAMME SCHEDULE

Day 1: 10th Nov-2025: Inaugural Session & Lecture Series:

*Session I: Inaugural Session **Chief Guest Principal (Dr. Satish Kumar Soni)***

Speaker: Dr. Akhil Bhardwaj, Department of Chemistry IISc Bangalore

Session II Speaker: Prof. Kalyan Sundar Ghosh, Department of Chemistry NIT Hamirpur

Session III Speaker: Dr. Manoj Sharma NCBS Bangalore & Azim Premji University

Session IV Speaker: Dr. Akhilesh Sharma; Hokkaido University, Sapporo Japan

Day 2: 11th Nov-2025: Foundations & Predictive Modeling in Chemistry

Theme: *Building the groundwork and applying ML for molecular prediction*

Session I: Introduction to AI in Chemistry (1.5 hrs) By Dr. Puneet R&D Expert

Session II: Data & Molecular Representation (2 hrs) By Dr. Puneet R&D Expert

Session III Speaker: Dr. Ankush Gupta; Coordinator INChO HBCSE Mumbai

Session IV: Hands-on Training: By Dr. Puneet R&D Expert E-Cell IIT Hyderabad

Day 3: 12th Nov-2025: Machine Learning & AI for Drug Discovery

Theme: *Applying ML to molecular prediction and docking*

Session I: Machine Learning for Chemistry (2.5 hrs) By Dr. Puneet R&D Expert

Session II: Hands-on Training: By Dr. Puneet R&D Expert

Session III: AI in Drug Discovery & Docking (3.5 hrs) By Dr. Puneet R&D Expert

Session IV: Hands-on Training: By Dr. Puneet R&D Expert

Day 4: 13th Nov-2025: Generative AI, Retrosynthesis & Capstone Project

Theme: *AI-driven molecule design and real-world applications*

Session I: Retrosynthesis & Generative AI (3 hrs)

Session II: Hands-on Training: By Dr. Puneet R & D Expert

Session III : Capstone Project & Presentations (3 hrs) By Dr. Puneet R&D Expert

Session IV: Team Project Evaluation By Dr. Puneet R&D Expert

A: Theme: : 1. Predict toxicity or solubility using ML models

2. AI-assisted docking for ligand identification

3. Retrosynthesis planning for designed molecules

B. Mentor review and discussion of real-world impact and feedback session

Day 5: 14th Nov-2025: Lecture Series & Valedictory Function:

Session I Speaker: Dr. Bharti Gaur, HOD Department of Chemistry NIT Hamirpur

Session II Speaker: Dr. Ranbir Singh, Associate Professor, Department of Material Science & Technology IIT Mandi

Session III: Dr. Tirupati Chander Sharma; "Scientist E" TBRL DRDO Chandigarh

Session IV: Valedictory Ceremony & Certificate-Prize Distribution

Vote of Thanks (Jitender Thakur)



Organizing Committee

Assignments Assigned to Chemistry Department

Dr. Samjeet Singh Thakur

Faculty Coordinator & Certificate Management

Dr. Naisergik Deepika Khanna

Faculty Convener for Seminar

Dr. Monika Puri

Faculty Convener for Workshop

Ms. Anjna Kumari

Faculty Co-Convener for Seminar

Dr. Sapana Kumari

Faculty Co-Convener for Workshop

Dr. Hem Suman Jamwal

Faculty Co-Convener for All Financial Transactions

Mr. Pankaj Sharma

Technical Assistant in Computer Lab

Mr. Jitender Kumar & (Five Students)

Student Coordinator for Welcome and Vote of Thanks; Technical Help

Mr. Kewal Krishan & (Five Students)

Student Coordinator for Certificate, Refreshment

**Chief Patron: Dr. Satish Kumar Soni
Principal NSCBM GC Hamirpur**

Patrons-cum-Session Chairpersons

Ms. Neelam Guleria; HOD Physics

Dr. Vijay Kumar Thakur; HOD Botany

Dr. Krishan Lal; HOD Zoology

Dr. Sanjay Kango; HOD Mathematics

Mr. Praveen Kumar; HOD Computer Science

Media Coordinator: Mr. Saurabh Sood; HOD JMC

Lab Assistant-cum-Refreshment Assistant

Mr. Banit Kumar Guleria

Mr. Kushal Kumar



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Audience: All Chemistry Faculty & MSc & BSc Chemistry Students.

Venue: Room No. 43 & BCA Computer Lab

Timing: 10: 30 am to 4: 00 pm for 10th November & 14th November 2025
& 9: 30 am to 4: 30 pm for 11th ; 12th and 13th November 2025

Workshop Fee: ₹ 1500/- for Each Participant

Account Number: 141822010001130

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